

Minimax determination of the energy spectrum of the Dirac equation in a Schwarzschild background

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Abstract

We calculate the bound-state energy spectrum of the Dirac Equation in a Schwarzschild black hole background using a minimax variational method. Our method extends that of Talman [1] to the case of non-Hermitian interactions, such as a black hole. The trial function is expressed in terms of a basis set that takes into account both the Hermitian limit of the interaction in the non-relativistic approximation, and the general behaviour of the solutions at the origin, the horizon and infinity. Using this trial function an approximation to the full complex energy bound-state spectrum is computed. We study the behaviour of the method as the coupling constant of the interaction is increased, which increases both the relativistic effects and the size of the non-Hermitian part of the interaction. Finally we confirm that the method follows the expected Hylleraas–Undheim behaviour.

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1 Introduction

Variational methods are an important practical technique for determining the eigenvalues of Hamiltonian operators. The methods aim to provide an approximation to the energy eigenvalues by the variation of the Rayleigh quotient

$$E_\phi = \frac{(\phi, \mathbf{H} \phi)}{(\phi, \phi)} \quad (1)$$

for a continuous set of trial functions $\phi = \phi(a)$. In non-relativistic quantum mechanics the energy spectrum is bounded from below and a simple minimization of E_ϕ with respect to a leads to an upper bound to the ground state energy. Furthermore, if ϕ is expressed on a finite-basis expansion, then the eigenvalues of H on this basis are approximations to the higher energy eigenvalues. This is known as the Hylleraas–Undheim theorem [2, 3].

For the Dirac equation the picture is more complicated as the spectrum of the Dirac Hamiltonian is not bounded from below. That is, the Hamiltonian allows states with positive and negative energy. Therefore, a direct minimization of the parameter a takes E_ϕ to $-\infty$. This is known as variational collapse [4]. Many different techniques have been devised to avoid this problem (for a review of the field, see [5]). Drake and Goldman [7] showed that for a well chosen basis the variational approach for the hydrogen atom leads to sensible results. They found that the energy eigenvalues split into one positive and one negative set. The positive set give the bound-state energies, while the

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negative energies are smaller than minus the electron's rest mass. Talman [1] explained how the finite basis expansion of the large and small parts of the trial solution provide the positive and negative eigen-energies respectively. Talman also addressed Grant's argument [8] that the variational collapse is caused by the incompleteness of the small-component basis. Talman discussed how the ground-state energy of a truncated small-component basis is a lower bound for the energy of a complete basis. It also turns out that this complete basis energy is an upper-bound for the exact energy. Dolbeault *et al.* [5] have proved that equation (3) below can be derived from a general variational principle, and have stressed that the difficulty in Talman's approach is to determine for which class of Hamiltonians it is valid. In particular, they have proved that the approach is valid for Hermitian Hamiltonians with potentials of the form $|r|^{-\beta}$, where $\beta \in (0, 1)$, which evidently include the Coulomb interaction.

Recently the bound-state spectrum of an electron in a Schwarzschild black hole back ground has been determined [10]. One of its main features is that the energy eigenvalues are complex, since the black hole interaction is non-Hermitian. The imaginary part of the energy eigenvalues gives the decay rate with time of the corresponding eigenstate. Furthermore, the state spectrum resembles that of the hydrogen atom for a small coupling constant. As the coupling constant is reduced, the imaginary part of the energy tends to zero as the interaction tends to one of Coulomb type. This offers a starting point to explore the variational methods for non-Hermitian Hamiltonians. In this paper we thus implement a minimax method based on Talman's approach for the black hole interaction. This method allows us to calculate the full complex energy eigenvalues and explore its behaviour with an increasing coupling constant. The approach developed here should have applications in a range of fields where one is forced to deal with non-Hermitian interactions, including the important subject of open systems.

2 Talman's minimax method

Talman's variational formulation for the energy eigenvalues follows from the decomposition of the Dirac wavefunction into its large and small parts. Following Grant [8], the two-component radial Dirac equation can be written as

$$\mathbf{H} \begin{pmatrix} g \\ f \end{pmatrix} = \begin{pmatrix} 1 + \frac{1}{mc^2} H_1(r) & \frac{\hbar}{mc} \frac{k-1}{r} - \frac{\hbar}{mc} \partial_r \\ \frac{\hbar}{mc} \frac{k+1}{r} + \frac{\hbar}{mc} \partial_r & -1 + \frac{1}{mc^2} H_1(r) \end{pmatrix} \begin{pmatrix} g \\ f \end{pmatrix} = \frac{E}{mc^2} \begin{pmatrix} g \\ f \end{pmatrix} \quad (2)$$

where $H_1(r)$ is the interaction term. The ground state energy can be obtained from the variation of the correct eigenfunction ϕ , determined by f and g ;

$$E = \min_g \left[\max_f \frac{(\phi, \mathbf{H} \phi)}{(\phi, \phi)} \right], \quad (3)$$

where ϕ is the two-component radial spinor

$$\phi(r) = \begin{pmatrix} g(r) \\ f(r) \end{pmatrix}. \quad (4)$$

If g is an arbitrary function, the maximum over f yields an upper-bound to the exact ground energy. The trial function ϕ can be expanded in a finite function

basis in the form

$$\phi(r) = \sum_{j=1}^n \begin{pmatrix} b^j g_j(r) \\ a^j f_j(r) \end{pmatrix}. \quad (5)$$

After a substitution of this function into equation (3), the minimax approximation is reduced to minimize E for each b^j and maximize it for each a^j . If we then consider vectors of the form

$$\alpha = (b_1 \dots b_n, a_1, \dots a_n)^t, \quad (6)$$

then the minimax variation of E leads to a generalized eigenvalue problem. This can be written

$$\mathbf{h} \alpha = E \mathbf{O} \alpha. \quad (7)$$

Here \mathbf{h} is a $(2n \times 2n)$ matrix

$$\mathbf{h} = \begin{pmatrix} \mathbf{h11}_{n \times n} & \mathbf{h12}_{n \times n} \\ \mathbf{h21}_{n \times n} & \mathbf{h22}_{n \times n} \end{pmatrix} \quad (8)$$

where the $(n \times n)$ matrices are given by

$$\mathbf{h11}_{lj} = \int_0^\infty g_l^* \mathbf{H}_{11} g_j r^2 dr \quad (9)$$

$$\mathbf{h12}_{lj} = \int_0^\infty g_l^* \mathbf{H}_{12} f_j r^2 dr \quad (10)$$

$$\mathbf{h21}_{lj} = \int_0^\infty f_l^* \mathbf{H}_{21} g_j r^2 dr \quad (11)$$

$$\mathbf{h22}_{lj} = \int_0^\infty f_l^* \mathbf{H}_{22} f_j r^2 dr. \quad (12)$$

The matrix \mathbf{O} is also a $(2n \times 2n)$ matrix given by the overlap integrals of the g_l and f_j . Its first $(n \times n)$ sub-matrix is

$$\mathbf{O11}_{lj} = \int_0^\infty g_l^* g_j r^2 dr, \quad (13)$$

with $\mathbf{O22}$ containing the equivalent f_j integrals, and all other terms vanishing.

Talman shows that for the Coulomb interaction the positive eigenvalues in equation (7) tend to the first energy eigenvalues as n increases, following a Hylleraas–Undheim behaviour.

3 Black hole interaction

The interaction H_1 for a black hole is given by [11]

$$\frac{1}{mc^2} H_1(r) = i \frac{\hbar}{mc} \sqrt{\frac{\hbar}{mcr} \frac{2GMm}{c\hbar}} \left(\partial_r + \frac{3}{4r} \right), \quad (14)$$

where the dimensional constants have been arranged into a convenient form. If we measure the radial distance in units of the Compton wavelength (mc/\hbar) we are left with the dimensionless coupling constant

$$\alpha = \frac{GMm}{c\hbar} \quad (15)$$

which gives the magnitude of the interaction. Using the interaction (14), we can now write the system of differential equations (2) in a more convenient form. With the change of variables

$$\varpi_1 = \frac{f}{r} \quad \text{and} \quad \varpi_2 = \frac{g}{r}, \quad (16)$$

the equations can be written as

$$\begin{pmatrix} \partial_r \varpi_1 \\ \partial_r \varpi_2 \end{pmatrix} = \mathbf{C}(r) \begin{pmatrix} \varpi_1 \\ \varpi_2 \end{pmatrix}, \quad (17)$$

where \mathbf{C} is the matrix

$$\mathbf{C}(r) = \frac{1}{r - 2\alpha} \begin{pmatrix} k - \frac{\alpha}{2r} + i\sqrt{2\alpha r}(1 + E) & i(-k - \frac{1}{4})\sqrt{\frac{2\alpha}{r}} + r(1 - E) \\ i(-k + \frac{1}{4})\sqrt{\frac{2\alpha}{r}} + r(1 + E) & -k - \frac{\alpha}{2r} - i\sqrt{2\alpha r}(1 - E) \end{pmatrix} \quad (18)$$

and we measure r and E in units of (mc/\hbar) and (mc^2) respectively. To simplify some of the later expressions we set the Compton wavelength mc/\hbar equal to 1.

Special attention must be given to the singularities of equation (17). The equation has three singular points. Two of them are regular singularities situated at the origin and at the horizon, $r = 2\alpha$. The third one is at infinity and is an irregular singularity of rank 2. Expansions of the solutions around the singular points provide the boundary conditions for the differential equations. The physical solutions are then selected from the correct boundaries at the singularities. Gathering the complete behaviour of the bound-state solution around the singular points, we obtain the general form

$$\psi(r) = R(r)e^{-\sqrt{1-E^2}r+2i\sqrt{2\alpha}rE} r^{\frac{\alpha(-1+2E^2)}{\sqrt{1-E^2}}} r^{-3/4}, \quad (19)$$

where $R(r)$ is an analytic function everywhere. The exponential factor and the first term in r take care of the singularity at infinity [12]. The $r^{-3/4}$ term corresponds to the boundary at the origin. The presence of this term is crucial as it accounts for the non-Hermiticity of the Hamiltonian [11]. This can be seen more explicitly from the calculation of the matrix elements of **h11** and **h22**. We find, for example, that

$$\begin{aligned} \mathbf{h11}_{lj} &= \int_0^\infty g_l^* g_j r^2 dr + \sqrt{2\alpha} \int_0^\infty g_l^* r^{3/4} i \partial_r (r^{3/4} g_j) dr \\ &= \left[\int_0^\infty g_j^* g_l r^2 dr \right]^* + \sqrt{2\alpha} \left[\int_0^\infty g_j^* r^{3/4} i \partial_r (r^{3/4} g_l^*) dr \right]^* \\ &\quad + i\sqrt{2\alpha} r^{3/2} g_l^* g_j|_0^\infty \\ &= \mathbf{h11}^*_{jl} + i\sqrt{2\alpha} r^{3/2} g_l^* g_j|_0^\infty. \end{aligned} \quad (20)$$

The second and third terms of the second equation follow from an integration by parts. A similar calculation holds for **h22**_{lj}. As a consequence, if there is at least one pair g_i and g_j where both tend to the origin as $r^{-3/4}$, the Hamiltonian is non-hermitian and the energy complex. The imaginary part of the energy is always negative and represents the decay rate of the wavefunction with time.

4 Minimax for the black hole interaction

Despite the fact that the interaction Hamiltonian is non-Hermitian, we can still apply the minimax approach, if we select a suitable function basis. The choice is based on the assumption that we achieve the non-relativistic limit for low α , in analogy with the Hydrogen atom. Lasenby *et al.* [10] show that the non-relativistic limits of the black hole and Coulomb interactions coincide. Therefore, we expect that the energy spectrum for the black hole resembles the Hydrogen spectrum for a low coupling constant. Restricting ourselves to the low coupling regime, the task is then to choose a finite function set that provides the Hydrogen properties and, at the same time, has the correct boundaries at the singularities.

From equation (19) we see that the bound state solutions of the Dirac equation must go as $r^{-3/4}$ for $r \rightarrow 0$, and as $e^{-br+i\beta\sqrt{r}}$ for $r \rightarrow \infty$. Taking these into account we define a set of discrete basis functions by

$$g_0 = e^{i\sqrt{2\alpha r}} e^{-br} r^{-\frac{3}{4}} \quad g_j = e^{i\sqrt{2\alpha r}} e^{-br} r^{j-1} \quad (21)$$

and

$$f_0 = e^{i\sqrt{2\alpha r}} e^{-ar} r^{-\frac{3}{4}} \quad f_j = e^{i\sqrt{2\alpha r}} e^{-ar} r^{j-1} \quad (22)$$

where $j = 1 \dots n$, and a and b are additional (nonlinear) parameters. We limit ourselves for the case where a and b are real. This corresponds to the condition $\Im(E) \ll \Re(E)$, expected for the non-relativistic limit. Note that we have increased the order of the approximation to $n + 1$ by including the extra terms g_0 and f_0 . From equation (20), the matrix \mathbf{h} will non-hermitian if we introduce g_0 and f_0 , and we find the the non-hermitian terms of \mathbf{h} from the quantities

$$\frac{\int_0^\infty g_0^* H_1(r) g_0 r^2 dr}{\int_0^\infty g_0^* g_0 r^2 dr} = -\alpha b - 4i\sqrt{\frac{\alpha}{\pi}} b^{\frac{3}{2}} \quad (23)$$

and

$$\frac{\int_0^\infty f_0^* H_1(r) f_0 r^2 dr}{\int_0^\infty f_0^* f_0 r^2 dr} = -\alpha a - 4i\sqrt{\frac{\alpha}{\pi}} a^{\frac{3}{2}}. \quad (24)$$

For the remaining terms down the diagonal of \mathbf{h} we find that

$$\int_0^\infty g_j^* H_1(r) g_j r^2 dr = - \int_0^\infty g_j^* \left(\frac{\alpha}{r} \right) g_j r^2 dr \quad (25)$$

with an identical result holding for f_j . We can see here the Coulomb interaction explicitly appearing in the diagonal of \mathbf{h} .

Leaving out the g_0 and f_0 terms in the expansion, the minimax method reduces to a real energy approximation. Thus, applying the minimax method to a pair of functions g_j and f_j with ($j \neq 0$) allows us to fix the values of a and b . With these values, the full basis can be determined, including the case $j = 0$. Our central assumption now is that equation (7) is remains valid, even when using the full basis set with \mathbf{h} non-Hermitian. The generalized eigenvalue problem of equation (7) allows us then to calculate complex eigen-energies. The validity of our assumption rests in part on the fact that the results obtained are in good agreement with the results of other, more accurate techniques. Since equation (7) can be derived from a variational principle of a Hermitian Hamiltonian, its validity for a non-Hermitian Hamiltonian suggests the existence of a variational principle for such a case.

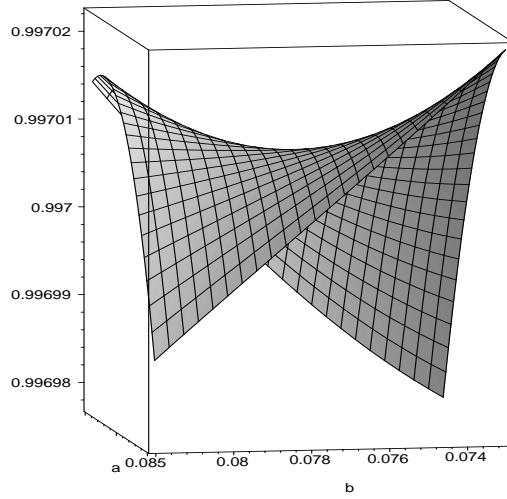


Figure 1: *Rayleigh quotient as function of the non-linear parameters a, b . $\alpha = 0.1$, $k = -1$; minimax at: $a = 8.9186905 \times 10^{-2}$, $b = 7.8238289 \times 10^{-2}$.*

5 Results

We start with the normalized basis function

$$\phi_* = \begin{pmatrix} 2b^{\frac{3}{2}} e^{i\sqrt{2\alpha}r} e^{-br} \\ 2a^{\frac{3}{2}} e^{i\sqrt{2\alpha}r} e^{-ar} \end{pmatrix}, \quad (26)$$

which sets $j = 1$ in equations (21) and (22). As discussed, the Rayleigh quotient for this function will be real. So the solution of equation (3) is given by the saddle point of E_ϕ as a function of a and b . An example of this saddle point is shown in figure 1. From equation (25) we see that the same result would have been obtained for this function basis had we used the the Coulomb interaction instead.

The values of a and b determine a unique function set specified by equations (21) and (22). A suitable trial function expanded on this function set is then

$$\phi_1 = e^{i\sqrt{2\alpha}r} \begin{pmatrix} e^{-br} \left(b^0 r^{-3/4} + \sum_{j=1}^n b^j r^{j-1} \right) \\ e^{-ar} \left(a^0 r^{-3/4} + \sum_{j=1}^n a^j r^{j-1} \right) \end{pmatrix}. \quad (27)$$

With this trial function, the eigenvalues of equation (7) can be obtained. Since the function with power $-3/4$ in equation (27) gives rise to the non-Hermitian terms in \mathbf{h} , the eigenvalues are complex. The approximation to the ground state energy is then obtained from the eigenvalue with minimum positive real part. As the order of the expansion is increased, we expect the approximation to improve its accuracy and, in particular, tend to a limit. That this is indeed the case is confirmed in figure 2.

The minimax procedure offers only an approximation to the exact bound-state energies. The accuracy of the method depends on the chosen trial function. We consider two extra trial functions and compare their results with a numerical

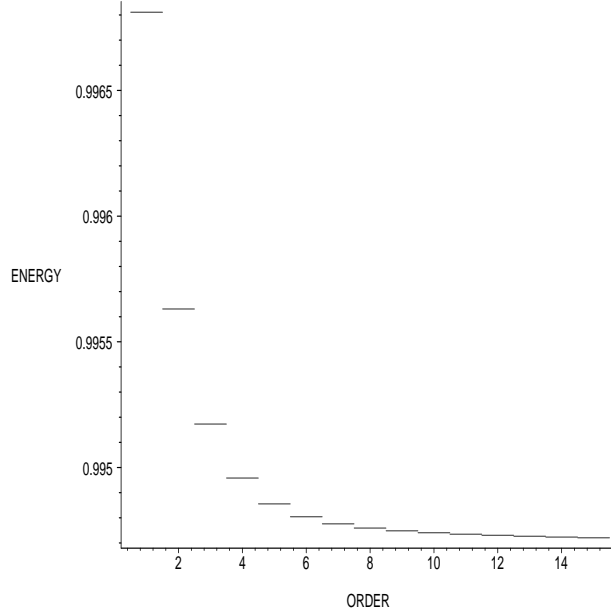


Figure 2: *Convergence to a single value of the approximation to the real part of the energy $\Re(E)$. For values $\alpha = 0.1, k = -1$, the energy $E/(mc^2) = 0.9947208 - i 2.0498160 \times 10^{-5}$ is obtained.*

shooting method that provides accurate values of the ground-state energy [10]. The shooting method finds the complex energies values for which the integrated solutions from the boundaries at the horizon and at infinity coincide. For the first trial function we consider the basis functions increasing on $1/4$ -rs powers of r . Then the trial function can be written as

$$\phi_2 = e^{i\sqrt{2\alpha}r} \begin{pmatrix} e^{-br} \left(\sum_{j=0}^n b^j r^{-\frac{3}{4} + \frac{j}{4}} \right) \\ e^{-ar} \left(\sum_{j=0}^n a^j r^{-\frac{3}{4} + \frac{j}{4}} \right) \end{pmatrix}. \quad (28)$$

For the second trial function we consider a combination of the trial functions in equations (27) and (28). The new trial function increases in $1/4$ powers for the negative powers of r and in integer values for positive powers. This is

$$\phi_3 = e^{i\sqrt{2\alpha}r} \begin{pmatrix} e^{-br} \left(\beta^0 r^{-\frac{3}{4}} + \beta^1 r^{-\frac{1}{2}} + \beta^3 r^{-\frac{1}{4}} + \sum_{j=0}^n b^j r^{\frac{j}{4}} \right) \\ e^{-ar} \left(\alpha^0 r^{-\frac{3}{4}} + \alpha^1 r^{-\frac{1}{2}} + \alpha^3 r^{-\frac{1}{4}} + \sum_{j=0}^n a^j r^{\frac{j}{4}} \right) \end{pmatrix}. \quad (29)$$

For $\alpha = 0.1, k = -1$, we find the ground-state energies given in table 1. (Note that the present conventions have k with opposite sign to the convention for κ in [10], so $k = -1$ is the ground state.) The table shows that the approximation to the real part of the complex energy given by the second trial function ($n = 16$) is extremely good, with the imaginary part also obtained quite accurately. The third trial function ($n = 18$) also gets the real part quite accurately, but the decay rate approximation is poor.

The trial function ϕ_2 is then more suitable for the study of the behaviour of the method with an increasing coupling constant. This is shown in figures 3

	$E/(mc^2)$
Trial function - minimax ϕ_1	$0.9947208 - i 2.0498160 \times 10^{-5}$
Trial function - minimax ϕ_2	$0.9946883 - i 2.7855588 \times 10^{-5}$
Trial function - minimax ϕ_3	$0.9946858 - i 3.0659648 \times 10^{-5}$
Shooting method	$0.9946882 - i 2.7870824 \times 10^{-5}$

Table 1: *Ground-state energy.* The energies are obtained from the minimax, using different trial functions, and from the shooting method.

and 4, where we can see that the minimax method gives good results for low couplings. Around the point of the last stable circular orbit $\alpha = 0.28$ [10] the minimax loses accuracy. This gives numerical indication that the region where the minimax works at its best is where classical circular orbits are still admissible.

The minimax method also provides approximations for the excited states. These are obtained from the other real positive eigenvalues. Using the trial function ϕ_3 a neat Hylleraas–Undheim behaviour is obtained for $\Re(E)$. This is shown in figures 5 and 6 where the real eigenstates tend to different energy levels as the order increases. In contrast to the hydrogen case, we have not only positive energy but also negative energy states. A selection of the values for the bound energies obtained in these figures are given in table 2, where the first two eigenvalues of positive and negative energies are compared for the cases $k = -1$ and $k = 1$, with $\alpha = 0.1$.

From this table we can extract a number of features. There is a spurious root for the first negative state with $k = 1$. All the other energies can be checked in a numerical integration routine and confirmed to give bound states. The solution for this spurious root does not show any structure other than an exponential divergence from the origin. The presence of spurious roots in variational methods for the Dirac equation is not new. In the past these roots have appeared from the study of the Coulomb interaction. In previous works, Drake and Goldman [7, 9] found the presence of a spurious root for the first eigenvalue of the case $k = 1$. In his original work [1] Talman showed how, for a particular case, the minimax method removes the spurious root found in [7]. Note that this kind of root is not present in table 2, so the minimax procedure has certainly excluded this case and given a sensible value for the first positive eigenvalue with $k = 1$. The spurious root is found, however, for the first negative eigenvalue of $k = 1$. This lies outside the scope of Talman’s arguments, since negative energy states of this type are not present in Coulomb interactions.

Another feature of table 2 is given by the comparison of the energies of

		Positive Energy/ mc^2	Negative Energy/ mc^2
$k = -1$	1 st	$0.994686 - i 3.06596 \times 10^{-5}$	$-0.998730 - i 1.53600 \times 10^{-8}$
	2 nd	$0.998698 - i 3.83240 \times 10^{-6}$	$-0.999437 - i 4.74152 \times 10^{-7}$
$k = 1$	1 st	$0.998731 - i 2.00712 \times 10^{-7}$	$-0.985823 - i 1.55033 \times 10^{-2}$
	2 nd	$0.999438 - i 5.22900 \times 10^{-8}$	$-0.994978 - i 1.75747 \times 10^{-3}$

Table 2: *Bound-state Energies for excited states*

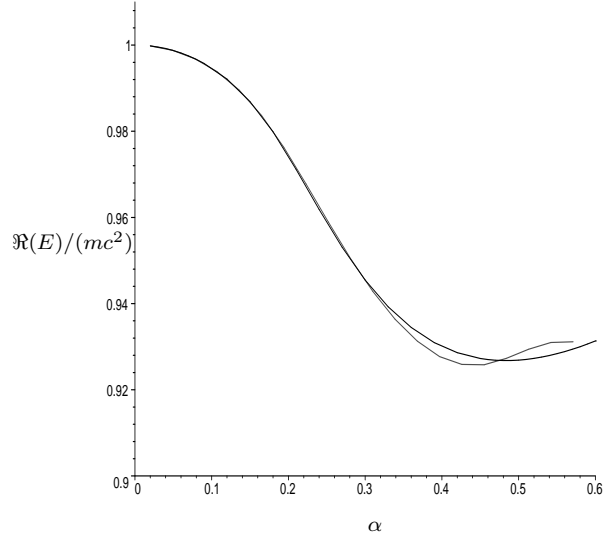


Figure 3: *Real part of the energy as a function of the black hole mass.* The real part of the energy given by the minimax (light hue) and by the shooting energy (dark hue) are compared for the ground state with $k = -1$.

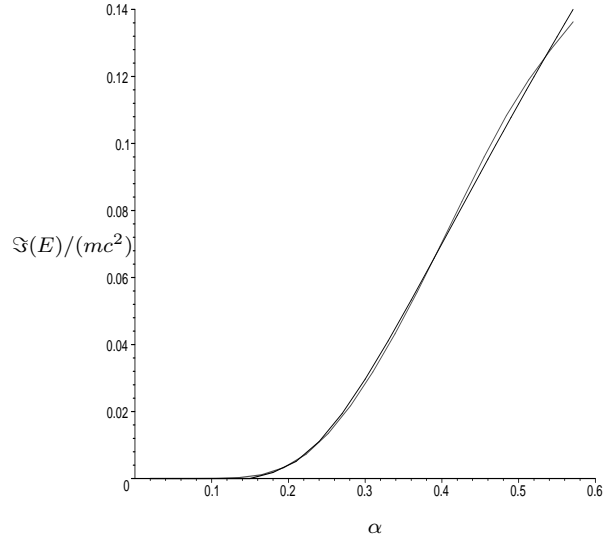


Figure 4: *Decay rate as a function of the black hole mass.* The decay rates given by the minimax (light hue) and the shooting (dark hue) corresponding to figure 3.

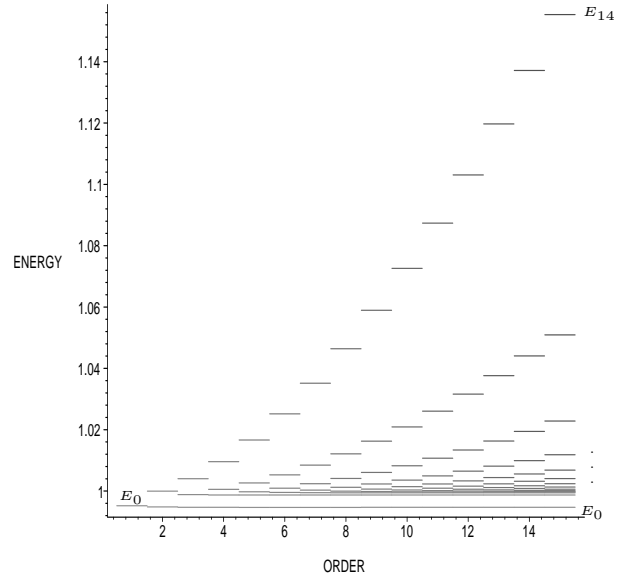


Figure 5: *Hylleraas-Undheim behaviour of the positive real part of the eigen-energies*, given the values $\alpha = 0.1$, $k = -1$ and the trial function (29).

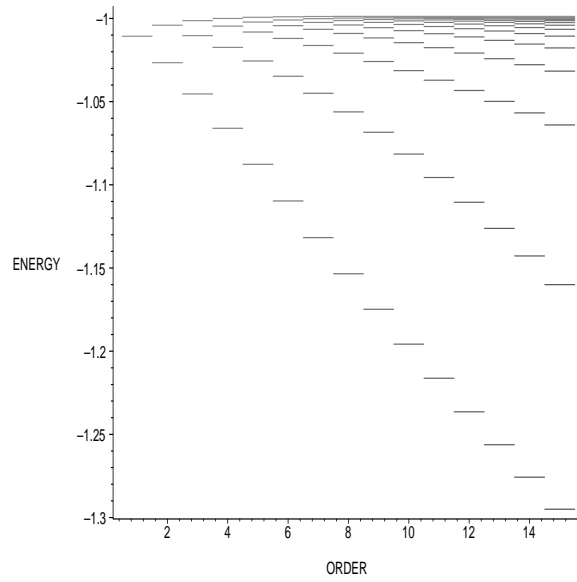


Figure 6: *Hylleraas-Undheim of the negative real part of the eigen-energies*, given the values $\alpha = 0.1$, $k = -1$ and the trial function (29).

the states $2S_{1/2}$ ($2^{nd}, k = -1$) and $2P_{1/2}$ ($1^{st}, k = 1$). For the low value of α used here, we see that the states have comparable energy, as is the case for the Coulomb interaction. At higher values of α for the gravitational interaction this degeneracy of the energy in the sign of k is lifted [10].

A further property we can extract from table 2 is the presence of charge conjugation symmetry. For a given state we should find another with opposite sign for both the real part of the energy and k , but with the same decay rate. This can be seen from the comparison between the real part of the state ($1^{st}, k = -1$) of positive energy and the state ($2^{nd}, k = 1$) of negative energy, as well as the comparison between the states of positive energy ($1^{st}, k = 1$), ($2^{nd}, k = 1$) and the states of negative energy ($1^{st}, k = -1$), ($2^{nd}, k = -1$) respectively. It is a bit disappointing that the imaginary energies of corresponding states have not the same value, as is required by the charge conjugation symmetry. This suggests that the minimax method will need to be further refined to find a more precise decay rates for the excited states.

6 Conclusions

The minimax method has proven to be a useful tool for analyzing the electron bound state energy spectrum in a black hole background. We have seen how the method works well not only for the small coupling limit but also sheds some light on what happens beyond the last classically stable circular orbit. The validity of the method suggests that the complex energy spectrum of the black hole can be obtained from a general variational principle.

The minimax method can only give an approximation to the exact energy. As we have seen this depends critically on the trial function used. Furthermore, we found that the method ceases to give reliable results around $\alpha \sim 0.4$, which may limit the applicability of the minimax method. One reason for this failure may be that we have assumed that the imaginary part of the energy is small as compared to the real part. This is no longer the case around $\alpha \sim 0.4$ for the $1S$ state. However, we may expect that the minimax method will continue to give accurate results for higher angular momentum states beyond $\alpha \sim 0.4$.

A further improvement of the minimax method can be given by the relaxation of the condition on the imaginary energy. As a consequence, the nonlinear parameters a and b could be considered as complex numbers. It then would be interesting to see whether this gives any improvements in either the determination of the energy for higher values of the black hole mass, or to the accuracy of the decay rates for excited states. Extending this method to larger values of α is a particularly significant problem, as the shooting method runs into numerical difficulties beyond α of around 6, whereas values of astrophysical interest start at around 10^{15} .

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